



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 145969

TO: Ben Sackey
Location: 5c31/5c18
Art Unit: 1626
Monday, February 28, 2005

Case Serial Number: 10/684726

From: Noble Jarrell
Location: Biotech-Chem Library
Rem 1B71
Phone: 272-2556

Noble.jarrell@uspto.gov

Search Notes

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STRUCTURE FILE UPDATES: 27 FEB 2005 HIGHEST RN 838819-79-7
DICTIONARY FILE UPDATES: 27 FEB 2005 HIGHEST RN 838819-79-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

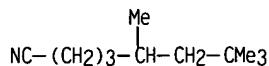
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d ide 113

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN 681449-57-0 REGISTRY
CN Octanenitrile, 5,7,7-trimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H21 N
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA Cplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP
(Properties); USES (Uses)



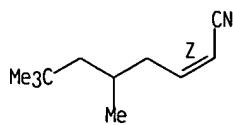
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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L26 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 681449-58-1 REGISTRY
CN 2-Octenenitrile, 5,7,7-trimethyl-, (2Z)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H19 N
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA Cplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.

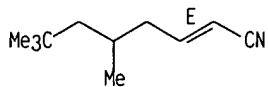


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1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L26 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 29898-30-4 REGISTRY
 CN 2-Octenenitrile, 5,7,7-trimethyl-, (2E)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 2-Octenenitrile, 5,7,7-trimethyl-, (E)- (8CI)
 FS STEREOSEARCH
 MF C11 H19 N
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
 DT.CA Caplus document type: Patent
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.

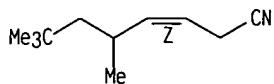


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L26 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 29680-30-6 REGISTRY
 CN 3-Octenenitrile, 5,7,7-trimethyl-, (3Z)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 3-Octenenitrile, 5,7,7-trimethyl-, (Z)- (8CI)
 FS STEREOSEARCH
 MF C11 H19 N
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, SPECINFO, USPATFULL
 DT.CA Caplus document type: Patent
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



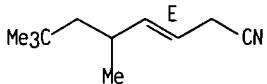
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L26 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 29680-29-3 REGISTRY

CN 3-Octenenitrile, 5,7,7-trimethyl-, (3E)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 3-Octenenitrile, 5,7,7-trimethyl-, (E)- (8CI)
 FS STEREOSEARCH
 MF C11 H19 N
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, SPECINFO, USPATFULL
 DT.CA Cplus document type: Patent
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> => => d ide 120 38

L20 ANSWER 38 OF 38 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 372-09-8 REGISTRY
 CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 2-Cyanoacetic acid
 CN Cyanoacetic acid
 CN Cyanoethanoic acid
 CN Malonic mononitrile
 CN Monocyanooacetic acid
 CN NSC 5571
 FS 3D CONCORD
 MF C3 H3 N 02
 CI COM
 LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS,
 CA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX,
 CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, GMELIN*,
 HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS,
 NIOSHTIC, PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE,
 TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)
 DT.CA Cplus document type: Conference; Dissertation; Journal; Patent; Report
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);
 CMBI (Combinatorial study); PREP (Preparation); PROC (Process); PRP
 (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in
 record)
 RLD.P Roles for non-specific derivatives from patents: BIOL (Biological
 study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent);
 USES (Uses)
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological
 study); CMBI (Combinatorial study); FORM (Formation, nonpreparative);
 OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties);
 RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
 RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical
 study); PREP (Preparation); PROC (Process); PRP (Properties); RACT
 (Reactant or reagent); USES (Uses)

NC-CH₂-CO₂H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1728 REFERENCES IN FILE CA (1907 TO DATE)
 81 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 1730 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 38 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his

(FILE 'HOME' ENTERED AT 11:27:15 ON 28 FEB 2005)

FILE 'HCAPLUS' ENTERED AT 11:28:03 ON 28 FEB 2005

L1 1 US20040127394/PN
 E DE2002-10247966/AP,PRN
 L2 1 DE2002-10247966/AP,PRN
 L3 1 L1-2

FILE 'REGISTRY' ENTERED AT 11:28:48 ON 28 FEB 2005

FILE 'HCAPLUS' ENTERED AT 11:28:49 ON 28 FEB 2005
 L4 TRA L3 1- RN : 9 TERMS

FILE 'REGISTRY' ENTERED AT 11:28:49 ON 28 FEB 2005
 L5 9 SEA L4

FILE 'WPIX' ENTERED AT 11:28:52 ON 28 FEB 2005
 L6 1 US20040127394/PN
 E DE2002-10247966/AP,PRN
 L7 1 DE2002-10247966/AP,PRN
 L8 1 L6-7

FILE 'REGISTRY' ENTERED AT 11:55:41 ON 28 FEB 2005
 L9 1399 C11H21N
 L10 QUE (PMS OR MAN OR IDS)/CI OR COMPD OR COMPOUND OR UNSPECIFIED
 L11 1275 L9 NOT L10
 L12 5 L11 AND OCTANENITRILE
 SEL 2
 DEL SEL
 SEL RN L12 2
 L13 1 E1 AND L12
 L14 1844 C9H18O
 L15 1582 L14 NOT L10
 L16 18 L15 AND OCTANAL
 L17 199 C3H3N02
 L18 126 L17 NOT L10
 L19 45 L18 AND ACETIC (1A)ACID
 L20 38 L19 AND CYANO
 L21 1231 C11H19N
 L22 1146 L21 NOT L10
 L23 112 L22 AND NITRILE
 L24 15 L23 AND OCTENENITRILE
 L25 13 L24 AND (2 OR 3) (1A) OCTENENITRILE
 SEL RN 1 10-12 L25
 L26 4 E2-5 AND L25

FILE 'HCAPLUS' ENTERED AT 12:27:07 ON 28 FEB 2005
 L27 1 L13
 L28 4 L26 OR OCTENENITRILE (3A) TRIMETHYL
 L29 3655 L20 OR ACETIC (1A) ACID (1A) CYANO OR (?CYANOACETIC/BI OR CYANO

L30 1 L29 AND L28
 L31 1 L27 AND L28
 L32 1 L27 OR L30 OR L31

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FILE COVERS 1907 - 28 Feb 2005 VOL 142 ISS 10
 FILE LAST UPDATED: 27 Feb 2005 (20050227/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all fhitstr 132 tot

L32 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2004:348009 HCAPLUS
 DN 140:356957
 ED Entered STN: 29 Apr 2004
 TI Preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and **isononylaldehyde** followed by catalytic hydrogenation
 IN Panten, Johannes; Fahlbusch, Karl-Georg; Werner, Matthias; Sillon, Pascal
 PA Symrise GmbH & Co. KG, Germany
 SO Eur. Pat. Appl., 7 pp.
 CODEN: EPXXDW
 DT Patent
 LA German
 IC ICM C07C255-03
 ICS A61K007-46
 CC 23-19 (Aliphatic Compounds)
 Section cross-reference(s): 46. 62

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1413570	A1	20040428	EP 2003-22338	20031004
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	DE 10247966	A1	20040506	DE 2002-10247966	20021015
	US 2004127394	A1	20040701	US 2003-684726	20031014
	BR 2003004488	A	20040831	BR 2003-4488	20031014
	JP 2004137275	A2	20040513	JP 2003-354687	20031015
PRAI	DE 2002-10247966	A	20021015		

CLASS

	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP	1413570	ICM	C07C255-03
		ICS	A61K007-46
EP	1413570	ECLA	C07C255/03

DE 10247966 ECLA C07C255/03
 US 2004127394 ECLA C07C255/03
 JP 2004137275 FTERM 4H003/AB27; 4H003/AC15; 4H003/BA12; 4H003/EA21;
 4H003/EB12; 4H003/ED02; 4H003/EE08; 4H003/FA26;
 4H006/AA01; 4H006/AA03; 4H006/AB14; 4H059/BA44;
 4H059/DA09; 4H059/EA35

AB Fragrant 5,7,7-trimethyloctanenitrile, useful as a fragrance in bleaches, is prepared in high yield and selectivity via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde to give the mixed-isomer intermediate **Z/E-5,7,7-Trimethyl-2(3)-octenenitriles** which are then subjected to catalytic (e.g., Pd/C) hydrogenation.

ST trimethyloctanenitrile fragrance prepn

IT Nitriles, preparation
 RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (aliphatic, 5,7,7-trimethyloctanenitrile: preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde followed by catalytic hydrogenation)

IT Knoevenagel reaction
 (of **cyanoacetic acid** and isononylaldehyde to give the mixed-isomer intermediate **Z/E-5,7,7-Trimethyl-2(3)-octenenitriles**)

IT Hydrogenation
 (of the mixed-isomer intermediate **Z/E-5,7,7-Trimethyl-2(3)-octenenitriles** into 5,7,7-trimethyloctanenitrile)

IT Odor and Odorous substances
 (preparation of 5,7,7-trimethyloctanenitrile as)

IT Bleaching agents
 Perfumes
 (preparation of fragrant 5,7,7-trimethyloctanenitrile for use in)

IT Hypochlorites
 RL: RGT (Reagent); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
 (preparation of fragrant 5,7,7-trimethyloctanenitrile for use in bleaches containing)

IT Nitriles, preparation
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (unsatd., **Z/E-5,7,7-Trimethyl-2(3)-octenenitriles**: preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde followed by catalytic hydrogenation of)

IT 29680-29-3P 29680-30-6P 29898-30-4P
 681449-58-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate: preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde followed by catalytic hydrogenation)

IT 7782-50-5. Chlorine, reactions
 RL: RGT (Reagent); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
 (preparation of fragrant 5,7,7-trimethyloctanenitrile for use in bleaches containing)

IT 681449-57-0P
 RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of **cyanoacetic acid** and isononylaldehyde followed by catalytic hydrogenation)

IT 372-09-8. **Cyanoacetic acid** 1333-74-0.
 Hydrogen, reactions 49824-43-3. Isononylaldehyde
 RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Anic Spa: GB 1523028 A 1978 HCPLUS
- (2) Bush Boake Allen Ltd: EP 0017396 A 1980 HCPLUS
- (3) Int Flavors & Fragrances Inc: EP 0347596 A 1989 HCPLUS
- (4) Unilever Plc: EP 0074253 B 1983 HCPLUS

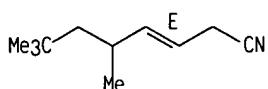
IT 29680-29-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)

RN 29680-29-3 HCPLUS

CN 3-Octenenitrile, 5,7,7-trimethyl-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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=> d his

(FILE 'HOME' ENTERED AT 11:27:15 ON 28 FEB 2005)

FILE 'HCAPLUS' ENTERED AT 11:28:03 ON 28 FEB 2005

L1 1 US20040127394/PN
E DE2002-10247966/AP,PRN
L2 1 DE2002-10247966/AP,PRN
L3 1 L1-2

FILE 'REGISTRY' ENTERED AT 11:28:48 ON 28 FEB 2005

FILE 'HCAPLUS' ENTERED AT 11:28:49 ON 28 FEB 2005
L4 TRA L3 1- RN : 9 TERMS

FILE 'REGISTRY' ENTERED AT 11:28:49 ON 28 FEB 2005
L5 9 SEA L4

FILE 'WPIX' ENTERED AT 11:28:52 ON 28 FEB 2005
L6 1 US20040127394/PN
E DE2002-10247966/AP,PRN
L7 1 DE2002-10247966/AP,PRN
L8 1 L6-7

=> b hcap

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FILE COVERS 1907 - 28 Feb 2005 VOL 142 ISS 10
FILE LAST UPDATED: 27 Feb 2005 (20050227/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all 13

L3 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:348009 HCAPLUS
DN 140:356957
ED Entered STN: 29 Apr 2004
TI Preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononyalaldehyde followed by catalytic hydrogenation
IN Panten, Johannes; Fahlbusch, Karl-Georg; Werner, Matthias; Sillon, Pascal
PA Symrise GmbH & Co. KG, Germany
SO Eur. Pat. Appl. 7 pp.
CODEN: EPXXDW
DT Patent
LA German
IC ICM C07C255-03

ICS A61K007-46
 CC 23-19 (Aliphatic Compounds)
 Section cross-reference(s): 46, 62

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1413570	A1	20040428	EP 2003-22338	20031004 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	DE 10247966	A1	20040506	DE 2002-10247966	20021015 <--
	US 2004127394	A1	20040701	US 2003-684726	20031014 <--
	BR 2003004488	A	20040831	BR 2003-4488	20031014 <--
	JP 2004137275	A2	20040513	JP 2003-354687	20031015 <--
PRAI	DE 2002-10247966	A	20021015		<--

CLASS

	PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
	EP 1413570	ICM	C07C255-03	
		ICS	A61K007-46	
	EP 1413570	ECLA	C07C255/03	<--
	DE 10247966	ECLA	C07C255/03	<--
	US 2004127394	ECLA	C07C255/03	<--
	JP 2004137275	FTERM	4H003/AB27; 4H003/AC15; 4H003/BA12; 4H003/EA21; 4H003/EB12; 4H003/ED02; 4H003/EE08; 4H003/FA26; 4H006/AA01; 4H006/AA03; 4H006/AB14; 4H059/BA44; 4H059/DA09; 4H059/EA35	<--

AB Fragrant 5,7,7-trimethyloctanenitrile, useful as a fragrance in bleaches, is prepared in high yield and selectivity via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde to give the mixed-isomer intermediate Z/E-5,7,7-Trimethyl-2(3)-octenonitriles which are then subjected to catalytic (e.g., Pd/C) hydrogenation.

ST trimethyloctanenitrile fragrance prep

IT Nitriles, preparation

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 (aliphatic, 5,7,7-trimethyloctanenitrile; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)

IT Knoevenagel reaction
 (of cyanoacetic acid and isononylaldehyde to give the mixed-isomer intermediate Z/E-5,7,7-Trimethyl-2(3)-octenonitriles)

IT Hydrogenation
 (of the mixed-isomer intermediate Z/E-5,7,7-Trimethyl-2(3)-octenonitriles into 5,7,7-trimethyloctanenitrile)

IT Odor and Odorous substances
 (preparation of 5,7,7-trimethyloctanenitrile as)

IT Bleaching agents
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 (preparation of fragrant 5,7,7-trimethyloctanenitrile for use in)

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 RL: RGT (Reagent); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
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IT Nitriles, preparation
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 (unsatd., Z/E-5,7,7-Trimethyl-2(3)-octenonitriles; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation of)

IT 29680-29-3P 29680-30-6P 29898-30-4P 681449-58-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(intermediate; preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)

IT 7782-50-5, Chlorine, reactions

RL: RGT (Reagent); TEM (Technical or engineered material use); RACT

(Reactant or reagent); USES (Uses)

(preparation of fragrant 5,7,7-trimethyloctanenitrile for use in bleaches containing)

IT 681449-57-0P

RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)

IT 372-09-8, Cyanoacetic acid 1333-74-0, Hydrogen, reactions 49824-43-3,

Isononylaldehyde

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)

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=> b reg

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STRUCTURE FILE UPDATES: 25 FEB 2005 HIGHEST RN 838086-80-9

DICTIONARY FILE UPDATES: 25 FEB 2005 HIGHEST RN 838086-80-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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Crossover limits have been increased. See HELP CROSSOVER for details.

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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d ide 15 tot

L5 ANSWER 1 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 681449-58-1 REGISTRY

CN 2-Octenenitrile, 5,7,7-trimethyl-, (2Z)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H19 N

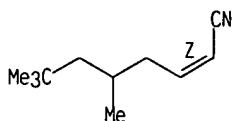
SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA Cplus document type: Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 681449-57-0 REGISTRY

CN Octanenitrile, 5,7,7-trimethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

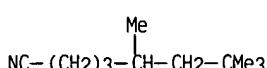
MF C11 H21 N

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA CAPplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 49824-43-3 REGISTRY

CN Octanal, 7-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 7-Methyloctanal

CN Isononylaldehyde

FS 3D CONCORD

MF C9 H18 O

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMLIST, CSCHEM, TOXCENTER, USPATFULL

(*File contains numerically searchable property data)

Other Sources: EINECS*

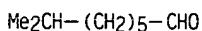
(**Enter CHEMLIST File for up-to-date regulatory information)

DT.CA CAPplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

RLD.P Roles for non-specific derivatives from patents: USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or reagent)

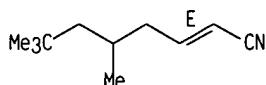


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

29 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 29 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 29898-30-4 REGISTRY
 CN 2-Octenenitrile, 5,7,7-trimethyl-, (2E)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 2-Octenenitrile, 5,7,7-trimethyl-, (E)- (8CI)
 FS STEREOSEARCH
 MF C11 H19 N
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL
 DT.CA Caplus document type: Patent
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.

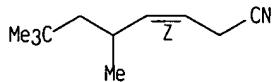


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 29680-30-6 REGISTRY
 CN 3-Octenenitrile, 5,7,7-trimethyl-, (3Z)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 3-Octenenitrile, 5,7,7-trimethyl-, (Z)- (8CI)
 FS STEREOSEARCH
 MF C11 H19 N
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, SPECINFO, USPATFULL
 DT.CA Caplus document type: Patent
 RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



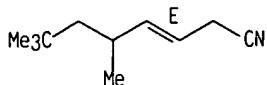
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 29680-29-3 REGISTRY
 CN 3-Octenenitrile, 5,7,7-trimethyl-, (3E)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 3-Octenenitrile, 5,7,7-trimethyl-, (E)- (8CI)
 FS STEREOSEARCH
 MF C11 H19 N
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, SPECINFO, USPATFULL
 DT.CA Caplus document type: Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 7782-50-5 REGISTRY

CN Chlorine (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN Chlorine mol.

CN Chlorine molecule (Cl2)

CN Diatomic chlorine

CN Dichlorine

CN Molecular chlorine

FS 3D CONCORD

MF C12

CI COM

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHM, CSNB, DDFU, DETHERM*, DIOGENES, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VETU, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

DT.CA Cplus document type: Book; Conference; Dissertation; Journal; Patent; Preprint; Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

C1-C1

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

68006 REFERENCES IN FILE CA (1907 TO DATE)

2274 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 68058 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 15 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 1333-74-0 REGISTRY
 CN Hydrogen (8CI, 9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN Dihydrogen
 CN Hydrogen (H2)
 CN Hydrogen molecule
 CN Mol. hydrogen
 CN Molecular hydrogen
 CN Orthohydrogen
 CN Parahydrogen
 CN Protium
 DR 725200-57-7
 MF H2
 CI COM
 LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABAB, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHM, CSNB, DDFU, DETHERM*, DIOGENES, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)
 DT.CA CAPLUS document type: Book; Conference; Dissertation; Journal; Patent; Preprint; Report
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
 RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
 RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

H-H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

295509 REFERENCES IN FILE CA (1907 TO DATE)
 3621 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 295705 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 372-09-8 REGISTRY

CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2-Cyanoacetic acid

CN Cyanoacetic acid

CN Cyanoethanoic acid

CN Malonic mononitrile

CN Monocyanoacetic acid

CN NSC 5571

FS 3D CONCORD

MF C3 H3 N 02

CI COM

LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

DT.CA Cplus document type: Conference; Dissertation; Journal; Patent; Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

NC-CH₂-CO₂H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1728 REFERENCES IN FILE CA (1907 TO DATE)

81 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1730 REFERENCES IN FILE CAPLUS (1907 TO DATE)

38 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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FILE LAST UPDATED: 24 FEB 2005 <20050224/UP>

MOST RECENT DERWENT UPDATE: 200513 <200513/DW>

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 HIT STRUCTURES WITHIN THE BIBLIOGRAPHIC DOCUMENT <<<

>>> SMILES and ISOSMILES strings are no longer available as
 Derwent Chemistry Resource display fields <<<

>>> THE CPI AND EPI MANUAL CODES HAVE BEEN REVISED FROM UPDATE 200501.
 PLEASE CHECK:
<http://thomsonderwent.com/support/dwpiref/reftools/classification/code-revision/>
 FOR DETAILS. <<<

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L8 ANSWER 1 OF 1 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
 AN 2004-358450 [34] WPIX
 DNC C2004-135920
 TI New compound 5,7,7-trimethyloctanonitrile useful for imparting an iris
 aroma to fragrance compositions and perfumed products, especially
 bleaches.
 DC D21 E16
 IN FAHLBUSCH, K; PANTEN, J; SILLON, P; WERNER, M
 PA (SYMR-N) SYMRIZE GMBH & CO KG; (DRAG-N) DRAGO CO GERBERDING CO GMBH;
 (FAHL-I) FAHLBUSCH K; (PANT-I) PANTEN J; (SILL-I) SILLON P; (WERN-I)
 WERNER M
 CYC 35
 PI EP 1413570 A1 20040428 (200434)* GE 7 C07C255-03
 R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LT LU LV
 MC MK NL PT RO SE SI SK TR
 DE 10247966 A1 20040506 (200434) C07C255-03
 JP 2004137275 A 20040513 (200434) 8 C07C255-03
 US 2004127394 A1 20040701 (200444) A61K007-46 <--
 BR 2003004488 A 20040831 (200460) A61K007-46
 CN 1502603 A 20040609 (200460) C07C255-03
 ADT EP 1413570 A1 EP 2003-22338 20031004; DE 10247966 A1 DE 2002-10247966
 20021015; JP 2004137275 A JP 2003-354687 20031015; US 2004127394 A1
 US 2003-684726 20031014; BR 2003004488 A BR 2003-4488 20031014; CN 1502603
 A CN 2003-1120359 20031015
 PRAI DE 2002-10247966 20021015
 IC ICM A61K007-46; C07C255-03
 ICS C07C255-02; C11B009-00; C11D003-395; C11D003-50; D06L003-00
 AB EP 1413570 A UPAB: 20041125
 NOVELTY - 5,7,7-Trimethyloctanonitrile (I) is new.
 DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for:
 (1) fragrance composition or perfumed article containing (I);
 (2) bleach composition comprising a bleaching agent, (I) and
 optionally conventional additives.
 USE - (I) is useful for imparting an iris aroma to fragrance
 compositions and perfumed products, especially bleaches based on chlorine
 and/or hypochlorite.
 ADVANTAGE - (I) has iris, vetiver, iris butter, woody and spicy aroma
 notes and has good stability in aggressive media, especially bleaches.
 Dwg. 0/0
 FS CPI
 FA AB: DCN
 MC CPI: D08-B12; D10-A05; E10-A15E

=> b home
FILE 'HOME' ENTERED AT 11:29:51 ON 28 FEB 2005

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